

Fundamental Conditions for N -th Order Accurate Lattice Boltzmann Models

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Abstract

In this paper, we theoretically prove a set of fundamental conditions pertaining discrete velocity sets and corresponding weights. These conditions provide sufficient conditions for *a priori* formulation of lattice Boltzmann models that automatically admit correct hydrodynamic moments up to any given N -th order.

Key words: Lattice Boltzmann, hydrodynamic moments

1. Introduction

Lattice Boltzmann methods (LBM) has been recognized as an advantageous numerical method for performing efficient computational fluid dynamics [1,2]. Not only it offers a new way of describing macroscopic fluid physics, but also it has become a practical computational tool and already has been making substantial impact in real world engineering applications [3]. Furthermore, according to a more recent interpretation, LBM models are special discrete approximations to the continuum Boltzmann kinetic equation [4,5]. Owing to such an underlying kinetic theory origin, LBM is expected to contain a wider range of fluid flow physics than the conventional hydrodynamic fluid descriptions [6,7,8,10]. The latter, such as the Euler or the Navier-Stokes equation, rely on various “theoretical” closure approximations for the non-equilibrium effects that are problematic when deviations from local thermodynamic equilibrium are no longer considered small. In addition, due to the fact that the fundamental turbulence modeling is built upon an analogy to regular fluid flows at finite Knudsen numbers, a kinetic theory representation is argued to be more suitable than the classical modeling approach of

modified Navier-Stokes equations [22]. However, how much the original range in kinetic theory can be retained depends on the order of accuracy in the LBM models used. Indeed, it has been shown that certain key physical effects beyond the Navier-Stokes equations can be accurately captured using higher order LBM models [5,9].

There have been extensive studies in LBM for more than a decade. However, popularly known LBM models are only accurate in the Navier-Stokes hydrodynamic regime (c.f., [12,14]). That is, physics higher than the Navier-Stokes order is contaminated by numerical artifacts in these LBM models. Furthermore, there has not been progress in systematically deriving higher order accurate LBM models until recently [5]. Originated from the framework of the so called Lattice Gas Automata [15,11], the conventional approach to formulating LBM models is based on a so called “top down” procedure. That is, giving a macroscopic equation such as the Euler or the Navier-Stokes equation, an LBM model may be constructed via an inverse Chapman-Enskog process and a *post-priori* parameter matching along with various subsequent “corrections” (cf., [13,14,16,17]). But more fundamentally, because such an approach relies on the availability of

macroscopic descriptions, it encounters an intrinsic difficulty in extending physics beyond the original macroscopic equations. It is well known that there is no well established and reliable macroscopic equation for deeper non-equilibrium physics beyond the Navier-Stokes regime.

One can theoretically show that the level of non-equilibrium physics is directly associated to the hydrodynamic moments [5]. Specifically, from the representation of the Chapman-Enskog expansion, there exists an apparent hierarchical relationship among hydrodynamic moments at various non-equilibrium levels. That is, n -th order hydrodynamic moments at m -th non-equilibrium level are related to the $(n+1)$ -th order moments at $(m-1)$ -th non-equilibrium level. Carrying out this hierarchy all the way, we see that in order to ensure the n -th moment physics at the m -th non-equilibrium level, it requires the equilibrium moments of $(m+n)$ -th order to be accurate. In other words, the higher order equilibrium hydrodynamic moments captured accurately, the wider range of non-equilibrium physics can be described. Indeed, the popularly known lattice Boltzmann models are only accurate up to the second order equilibrium moment (i.e., the equilibrium momentum flux tensor). As a result, these models only give an approximately correct “level-1 non-equilibrium momentum flux. This is a reason why the conventional LBM models are only applicable to the Navier-Stokes (Newtonian) fluid physics in low Mach number isothermal situations [11,12,13,14].

Based on the above, we see that the essential requirement for accurately capturing a wider range of physics is directly related to achieving equilibrium hydrodynamic moments to higher orders. Once the higher order moments are accurately realized, the resulting hydrodynamic equations such as the Euler, the Navier-Stokes and beyond are automatically attained. This is accomplished without the conventional *post-priori* procedure. As shown in this paper, the above requirement dictates a set of fundamental conditions on the supporting lattice velocity basis in LBM. That is, given an N -th order moment accuracy requirement, the set of fundamental conditions automatically defines the choice of a discrete lattice velocity set and its corresponding weights for such a purpose.

In this paper, we theoretically derive this set of fundamental conditions for LBM models of N -th order. We prove how the correct hydrodynamic moments up to the corresponding order are realized

once the conditions are satisfied.

2. Achieving Correct Hydrodynamic Moments via Discrete Velocities

According to the standard continuum Boltzmann kinetic theory, an n -th order equilibrium hydrodynamic moment tensor in D -dimension is defined as

$$\mathbf{M}^{(n)}(\mathbf{x}, t) \equiv \int d^D \mathbf{c} \underbrace{\mathbf{c} \mathbf{c} \cdots \mathbf{c}}_n f^{eq}(\mathbf{x}, \mathbf{c}, t) \quad (1)$$

Equivalently, it can be expressed in a Cartesian component form as follows,

$$M_{i_1, i_2, \dots, i_n}^{(n)}(\mathbf{x}, t) \equiv \int d^D \mathbf{c} c_{i_1} c_{i_2} \cdots c_{i_n} f^{eq}(\mathbf{x}, \mathbf{c}, t) \quad (2)$$

where subscripts i_1, i_2, \dots, i_n are Cartesian component indices. c_i is the i -th Cartesian component of the microscopic particle velocity \mathbf{c} . The equilibrium distribution has the standard Maxwell-Boltzmann form,

$$f^{eq}(\mathbf{x}, \mathbf{c}, t) = \frac{\rho(\mathbf{x}, t)}{[2\pi\theta(\mathbf{x}, t)]^{D/2}} \times \exp \left[-\frac{(\mathbf{c} - \mathbf{u}(\mathbf{x}, t))^2}{2\theta(\mathbf{x}, t)} \right] \quad (3)$$

where the macroscopic density, fluid velocity, and temperature are defined, respectively

$$\begin{aligned} \rho(\mathbf{x}, t) &= \int d^D \mathbf{c} f^{eq}(\mathbf{x}, \mathbf{c}, t) \\ \rho \mathbf{u}(\mathbf{x}, t) &= \int d^D \mathbf{c} \mathbf{c} f^{eq}(\mathbf{x}, \mathbf{c}, t) \\ D\rho\theta(\mathbf{x}, t) &= \int d^D \mathbf{c} (\mathbf{c} - \mathbf{u}(\mathbf{x}, t))^2 f^{eq}(\mathbf{x}, \mathbf{c}, t) \end{aligned} \quad (4)$$

Apparently, the above three relations correspond to the zero-th, first, and the trace of the second order hydrodynamic moments. It is well known that these three moments correspond to conservation laws and are invariant under any local collisions.

Notice the density ρ is an overall multiplier on all moments, without loss of generality for the subsequent analysis, we set it to unity.

Now let us define an analogous hydrodynamic moment expression in terms of summations over discrete velocity values below,

$$\tilde{\mathbf{M}}^{(n)}(\mathbf{x}, t) \equiv \sum_{\alpha=0}^b \underbrace{c_{\alpha} c_{\alpha} \cdots c_{\alpha}}_n f_{\alpha}^{eq}(\mathbf{x}, t) \quad (5)$$

Or equivalently, in a Cartesian component form

$$\tilde{M}_{i_1, i_2, \dots, i_n}^{(n)}(\mathbf{x}, t) \equiv \sum_{\alpha=0}^b c_{\alpha, i_1} c_{\alpha, i_2} \cdots c_{\alpha, i_n} f_{\alpha}^{eq}(\mathbf{x}, t) \quad (6)$$

In the above, we have assumed there are $b+1$ number of discrete D -dimensional vector values in the basis discrete velocity set: $\{\mathbf{c}_{\alpha} : \alpha = 0, \dots, b\}$. Similarly, we define an analogous equilibrium distribution function,

$$f_{\alpha}^{eq}(\mathbf{x}, t) = \bar{w}_{\alpha}(\theta(\mathbf{x}, t)) \exp \left[-\frac{(\mathbf{c}_{\alpha} - \mathbf{u}(\mathbf{x}, t))^2}{2\theta(\mathbf{x}, t)} \right] \quad (7)$$

where the macroscopic density, fluid velocity, and temperature are now defined in terms of moment summations instead,

$$\begin{aligned} 1 &= \sum_{\alpha=0}^b f_{\alpha}^{eq}(\mathbf{x}, t) \\ \mathbf{u}(\mathbf{x}, t) &= \sum_{\alpha=0}^b \mathbf{c}_{\alpha} f_{\alpha}^{eq}(\mathbf{x}, t) \\ D\theta(\mathbf{x}, t) &= \sum_{\alpha=0}^b (\mathbf{c}_{\alpha} - \mathbf{u})^2 f_{\alpha}^{eq}(\mathbf{x}, t) \end{aligned} \quad (8)$$

In the above, \bar{w}_{α} is a weighting factor that is at most dependent on $\theta(\mathbf{x}, t)$. Based on this fact, we can also re-express the discrete equilibrium distribution (7) in an alternative and simpler form:

$$\begin{aligned} f_{\alpha}^{eq} &= \bar{w}_{\alpha}(\theta) \exp \left[-\frac{(\mathbf{c}_{\alpha} - \mathbf{u})^2}{2\theta} \right] \\ &= w_{\alpha}(\theta) \exp \left[\frac{\mathbf{c}_{\alpha} \cdot \mathbf{u}}{\theta} \right] \exp \left[-\frac{\mathbf{u}^2}{2\theta} \right] \end{aligned} \quad (9)$$

by defining $w_{\alpha}(\theta) \equiv \bar{w}_{\alpha}(\theta) \exp[-\frac{\mathbf{u}^2}{2\theta}]$. Therefore, the discrete moment definition (6) can be re-expressed as,

$$\begin{aligned} \tilde{M}_{i_1, i_2, \dots, i_n}^{(n)} &\equiv \sum_{\alpha=0}^b c_{\alpha, i_1} c_{\alpha, i_2} \cdots c_{\alpha, i_n} w_{\alpha}(\theta) \\ &\times \exp \left[\frac{\mathbf{c}_{\alpha} \cdot \mathbf{u}}{\theta} \right] \exp \left[-\frac{\mathbf{u}^2}{2\theta} \right] \end{aligned} \quad (10)$$

Having all the basic definitions above specified, we are now ready to prove several fundamental conditions for a lattice velocity basis supporting an n -th order hydrodynamic moment accuracy and its corresponding form for the discrete equilibrium distribution function. These conditions are set forth for

measuring any given lattice in terms of an intrinsic tensor:

$$E_{i_1, \dots, i_n}^{(n)} \equiv \sum_{\alpha=0}^b w_{\alpha}(\theta) c_{\alpha, i_1} c_{\alpha, i_2} \cdots c_{\alpha, i_n} \quad (11)$$

Theorem 1 *Discrete moment $\tilde{\mathbf{M}}^{(n)}$ is equal to the moment $\mathbf{M}^{(n)}$ of the continuum Boltzmann kinetic theory, if the supporting lattice velocity basis satisfy the following conditions:*

$$E_{i_1, i_2, \dots, i_n}^{(n)} = \begin{cases} \theta^{n/2} \Delta_{i_1 i_2, \dots, i_n}^{(n)}, & n = 0, 2, 4, \dots \\ 0, & n = 1, 3, 5, \dots \end{cases} \quad (12)$$

In the above, $\Delta_{i_1, i_2, \dots, i_n}^{(n)}$ is the n -th order delta function defined as a summation of $n/2$ ($n = \text{even integer}$) products of simple Kronecker delta functions $\delta_{i_1 i_2} \cdots \delta_{i_{n-1} i_n}$ and those from distinctive permutations of its sub-indices [11,18,19,20]. There are $(n-1)!! \equiv (n-1) \cdot (n-3) \cdots 3 \cdot 1$ total number of distinctive terms in $\Delta_{i_1 i_2 \dots i_n}^{(n)}$. For instance, $\Delta_{ij}^{(2)} \equiv \delta_{ij}$, and

$$\begin{aligned} \Delta_{ijkl}^{(4)} &= \delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \\ \Delta_{ijklmn}^{(6)} &= \delta_{ij} \Delta_{klmn}^{(4)} + \delta_{ik} \Delta_{lmnj}^{(4)} + \delta_{il} \Delta_{mnlj}^{(4)} \\ &\quad + \delta_{im} \Delta_{njk l}^{(4)} + \delta_{in} \Delta_{jklm}^{(4)} \end{aligned} \quad (13)$$

Obviously, a lattice velocity set that satisfy condition (12) for $E^{(n)}$ is n -th order isotropic.

Proof of Theorem 1: First we prove for the zeroth order moment, $\tilde{\mathbf{M}}^{(0)} = \mathbf{M}^{(0)} = 1$. According to (9) we have,

$$\begin{aligned} \tilde{\mathbf{M}}^{(0)} &= \exp \left[-\frac{\mathbf{u}^2}{2\theta} \right] \sum_{\alpha=0}^b w_{\alpha} \exp \left[\frac{\mathbf{c}_{\alpha} \cdot \mathbf{u}}{\theta} \right] \\ &= \exp \left[-\frac{\mathbf{u}^2}{2\theta} \right] \sum_{l=0}^{\infty} \frac{1}{\theta^l l!} \sum_{\alpha=0}^b w_{\alpha} (\mathbf{c}_{\alpha} \cdot \mathbf{u})^l \end{aligned} \quad (14)$$

If (12) is satisfied, then all odd valued l terms vanish, and the even valued terms become,

$$\begin{aligned} \sum_{\alpha=0}^b w_{\alpha} (\mathbf{c}_{\alpha} \cdot \mathbf{u})^{2l} &= \theta^l \Delta^{(2l)} \otimes \underbrace{\mathbf{u} \mathbf{u} \cdots \mathbf{u}}_{2l} \\ &= (2l-1)!! \theta^l \mathbf{u}^{2l} \end{aligned} \quad (15)$$

In the above \otimes denotes a scalar product of two tensors. Therefore, (14) reduces to,

$$\begin{aligned}\tilde{\mathbf{M}}^{(0)} &= \exp \left[-\frac{\mathbf{u}^2}{2\theta} \right] \left\{ 1 + \sum_{l=1}^{\infty} \frac{(2l-1)!!}{(2l)!} \frac{\mathbf{u}^{2l}}{\theta^l} \right\} \\ &= \exp \left[-\frac{\mathbf{u}^2}{2\theta} \right] \left\{ 1 + \sum_{l=1}^{\infty} \frac{1}{l!} \frac{\mathbf{u}^{2l}}{(2\theta)^l} \right\}\end{aligned}\quad (16)$$

where the identity $(2l-1)!!/(2l)! = 2^{-l}/l!$ is used. Since,

$$1 + \sum_{l=1}^{\infty} \frac{1}{l!} \frac{\mathbf{u}^{2l}}{(2\theta)^l} = \exp \left[\frac{\mathbf{u}^2}{2\theta} \right] \quad (17)$$

Substituting this into (16), we have proved that $\tilde{\mathbf{M}}^{(0)} = 1$.

Next, we prove $\tilde{\mathbf{M}}^{(n)} = \mathbf{M}^{(n)}$ for $n > 0$. We start this by defining a partition function in discrete velocity space,

$$\mathcal{Q} \equiv \sum_{\alpha=0}^b w_{\alpha} \exp \left[\frac{\mathbf{c}_{\alpha} \cdot \mathbf{u}}{\theta} \right] = \exp \left[\frac{\mathbf{u}^2}{2\theta} \right] \quad (18)$$

Notice the second equality in the above is a result of the analysis of $\tilde{\mathbf{M}}^{(0)} = 1$. Consequently, we show that satisfying the second equality is a sufficient condition for achieving the correct hydrodynamic moment for any integer n . First of all, we have the following general relationship,

$$\begin{aligned}\tilde{\mathbf{M}}^{(n)} &= \exp \left[-\frac{\mathbf{u}^2}{2\theta} \right] \sum_{\alpha=0}^b w_{\alpha} \underbrace{\mathbf{c}_{\alpha} \mathbf{c}_{\alpha} \cdots \mathbf{c}_{\alpha}}_n \exp \left[\frac{\mathbf{c}_{\alpha} \cdot \mathbf{u}}{\theta} \right] \\ &= \exp \left[-\frac{\mathbf{u}^2}{2\theta} \right] \theta^n \frac{\partial^n}{\partial \mathbf{u}^n} \sum_{\alpha=0}^b w_{\alpha} \exp \left[\frac{\mathbf{c}_{\alpha} \cdot \mathbf{u}}{\theta} \right] \\ &= \exp \left[-\frac{\mathbf{u}^2}{2\theta} \right] \theta^n \frac{\partial^n}{\partial \mathbf{u}^n} \mathcal{Q}\end{aligned}\quad (19)$$

Since $\mathcal{Q} = \exp [\mathbf{u}^2/2\theta]$, then Eq. (19) becomes

$$\tilde{\mathbf{M}}^{(n)} = \exp \left[-\frac{\mathbf{u}^2}{2\theta} \right] \theta^n \frac{\partial^n}{\partial \mathbf{u}^n} \left[\exp \left(\frac{\mathbf{u}^2}{2\theta} \right) \right] \quad (20)$$

In comparison, from the continuum Boltzmann kinetic theory, we have

$$\begin{aligned}\mathbf{M}^{(n)} &= \frac{1}{(2\pi\theta)^{D/2}} \int d^D \mathbf{c} \underbrace{\mathbf{c} \cdots \mathbf{c}}_n \exp \left[-\frac{(\mathbf{c} - \mathbf{u})^2}{2\theta} \right] \\ &= e^{-\frac{\mathbf{u}^2}{2\theta}} \int d^D \mathbf{c} \underbrace{\mathbf{c} \cdots \mathbf{c}}_n (2\pi\theta)^{-\frac{D}{2}} e^{-\frac{\mathbf{c}^2}{2\theta} + \frac{\mathbf{c} \cdot \mathbf{u}}{\theta}} \\ &= e^{-\frac{\mathbf{u}^2}{2\theta}} \theta^n \frac{\partial^n}{\partial \mathbf{u}^n} \int d^D \mathbf{c} (2\pi\theta)^{-\frac{D}{2}} e^{-\frac{\mathbf{c}^2}{2\theta} + \frac{\mathbf{c} \cdot \mathbf{u}}{\theta}}\end{aligned}\quad (21)$$

It is easily shown that

$$\int d^D \mathbf{c} (2\pi\theta)^{-\frac{D}{2}} e^{-\frac{\mathbf{c}^2}{2\theta} + \frac{\mathbf{c} \cdot \mathbf{u}}{\theta}} = \exp \left[\frac{\mathbf{u}^2}{2\theta} \right]$$

Henceforth, we have shown that (21) and (20) have exactly the same form. Subsequently, we have proved the theorem that $\tilde{\mathbf{M}}^{(n)} = \mathbf{M}^{(n)}$ for any positive integer n , if condition (12) is satisfied.

It is revealing to check a few obvious representative examples. First of all, the first moment

$$\tilde{\mathbf{M}}^{(1)} = \exp \left[-\frac{\mathbf{u}^2}{2\theta} \right] \theta \frac{\partial}{\partial \mathbf{u}} \exp \left[\frac{\mathbf{u}^2}{2\theta} \right] = \mathbf{u}$$

This is simply the fluid momentum or the fluid velocity.

On the other hand, the second moment

$$\tilde{\mathbf{M}}^{(2)} = \exp \left[-\frac{\mathbf{u}^2}{2\theta} \right] \theta^2 \frac{\partial^2}{\partial \mathbf{u}^2} \exp \left[\frac{\mathbf{u}^2}{2\theta} \right] = \theta \mathbf{I} + \mathbf{u} \mathbf{u}$$

where \mathbf{I} is the second rank unity tensor. Hence the second moment has precisely the same form of the correct hydrodynamic momentum flux tensor. Furthermore, we have

$$\frac{1}{2} \text{Trace}(\tilde{\mathbf{M}}^{(2)}) = \frac{D}{2} \theta + \frac{1}{2} \mathbf{u}^2$$

which is exactly the hydrodynamic total energy.

3. Moment Accuracy for Lattices of Finite Isotropy

In the previous section, we have proved that condition (12) sufficiently ensures all moments defined via summations over discrete lattice velocity values are equal to that of the continuum Boltzmann kinetic theory. However, such a condition is unnecessarily too strong, because it requires the supporting lattice basis to have an infinite isotropy (i.e., $n \rightarrow \infty$). Obviously, no lattice velocity set containing a finite number of discrete values is able to meet such a requirement. Hence a realistic goal is to find a relationship between the hydrodynamic moments up to a given finite order and the corresponding isotropy for the supporting lattice velocity basis.

First of all, we notice the existence of a hierarchical relationship among the hydrodynamic moments. Based on definition (19), we have

$$\tilde{\mathbf{M}}^{(n)} = \exp \left[-\frac{\mathbf{u}^2}{2\theta} \right] \left(\theta \frac{\partial}{\partial \mathbf{u}} \right)^n \mathcal{Q} \quad (22)$$

Hence,

$$\begin{aligned}
\tilde{\mathbf{M}}^{(n+1)} &= \exp \left[-\frac{\mathbf{u}^2}{2\theta} \right] \theta \frac{\partial}{\partial \mathbf{u}} \left(\theta \frac{\partial}{\partial \mathbf{u}} \right)^n \mathcal{Q} \\
&= \exp \left[-\frac{\mathbf{u}^2}{2\theta} \right] \theta \frac{\partial}{\partial \mathbf{u}} \left[e^{\frac{\mathbf{u}^2}{2\theta}} e^{-\frac{\mathbf{u}^2}{2\theta}} \left(\theta \frac{\partial}{\partial \mathbf{u}} \right)^n \mathcal{Q} \right] \\
&= \exp \left[-\frac{\mathbf{u}^2}{2\theta} \right] \theta \frac{\partial}{\partial \mathbf{u}} \left[\exp \left(\frac{\mathbf{u}^2}{2\theta} \right) \tilde{\mathbf{M}}^{(n)} \right]
\end{aligned}$$

This gives the hierarchical relationship,

$$\tilde{\mathbf{M}}^{(n+1)} = \mathbf{u} \tilde{\mathbf{M}}^{(n)} + \theta \frac{\partial}{\partial \mathbf{u}} \tilde{\mathbf{M}}^{(n)} \quad (23)$$

Using the hierarchical relationship (23), all higher order moments are derivable starting from $\tilde{\mathbf{M}}^{(0)} = 1$. More importantly, we realize that n -th order moment $\tilde{\mathbf{M}}^{(n)}$ is an n -th order polynomial in terms of the power of the fluid velocity. That is, the highest power in $\tilde{\mathbf{M}}^{(n)}$ is \mathbf{u}^n . Since hydrodynamic moments up to a finite order only involve a finite power of fluid velocity, we expect moment accuracy up to a finite order can be achieved by a finite lattice set of adequate isotropy. Having established these properties, we arrive at the next theorem below.

Theorem 2 *If the supporting lattice velocity basis satisfies the following conditions*

$$E_{i_1, \dots, i_n}^{(n)} = \begin{cases} \theta^{n/2} \Delta_{i_1, \dots, i_n}^{(n)}, & n = 0, 2, \dots, 2N \\ 0, & n = \text{odd integer} \end{cases} \quad (24)$$

and if the discrete equilibrium distribution function $f_\alpha^{eq, (N)}$ is a truncation of the original exponential form by retaining terms only up to \mathbf{u}^N , then the discrete moment $\tilde{\mathbf{M}}^{(n)}$ is accurate and equal to the moment $\mathbf{M}^{(n)}$ of the continuum Boltzmann kinetic theory for any $n \leq N$. N is any given finite positive integer.

It is easily recognized that the basis lattice velocity set satisfying the above condition must be $2N$ -order isotropic (c.f., [11,24]).

Proof of Theorem 2: We start by first examining the standard Maxwell-Boltzmann distribution (3), and express it in an expanded form in powers of fluid velocity \mathbf{u} . This is very easily accomplished by taking advantage of the following generating function for Hermite series,

$$\exp [2tx - t^2] = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!} t^n \quad (25)$$

where $H_n(x)$ is the standard n -th order Hermite polynomial. Let us define the unity vector $\hat{\mathbf{u}} \equiv \mathbf{u}/|\mathbf{u}|$

and $|\mathbf{u}| \equiv \sqrt{\sum_{i=1}^D u_i^2}$ is the magnitude, and $\xi \equiv \mathbf{c} \cdot \hat{\mathbf{u}}/\sqrt{2\theta}$. We can formally express the distribution (3) as,

$$\begin{aligned}
f^{eq}(\mathbf{x}, \mathbf{c}, t) &= \frac{1}{(2\pi\theta)^{\frac{D}{2}}} \exp \left[-\frac{(\mathbf{c} - \mathbf{u})^2}{2\theta} \right] \\
&= \frac{1}{(2\pi\theta)^{\frac{D}{2}}} e^{-\frac{\mathbf{c}^2}{2\theta}} \exp \left[\frac{\mathbf{c} \cdot \mathbf{u}}{\theta} - \frac{\mathbf{u}^2}{2\theta} \right] \\
&= \frac{1}{(2\pi\theta)^{\frac{D}{2}}} e^{-\frac{\mathbf{c}^2}{2\theta}} \sum_{n=0}^{\infty} \frac{H_n(\xi)}{n!} \left(\frac{\mathbf{u}}{\sqrt{2\theta}} \right)^n \quad (26)
\end{aligned}$$

A truncated series $f^{eq, (N)}$ of the above can be defined by simply retaining the terms up to \mathbf{u}^N . Based on the orthogonal property of the Hermite polynomials, namely

$$\int_{-\infty}^{\infty} dx e^{-x^2} H_m(x) H_n(x) = 0; \quad \forall m \neq n \quad (27)$$

and because \mathbf{c} of power N can be fully represented by Hermite polynomials $\{H_n; n = 0, \dots, N\}$, it is straightforward to see that moments up to N -th order constructed out of f^{eq} are identical to that of $f^{eq, (N)}$, for the higher order terms in f^{eq} give vanishing contributions due to orthogonality.

Next, similar to the above, we expand the discrete distribution (9), and keeping terms only up to \mathbf{u}^N ,

$$\begin{aligned}
f_\alpha^{eq, (N)} &= w_\alpha \exp \left[\frac{\mathbf{c}_\alpha \cdot \mathbf{u}}{\theta} - \frac{\mathbf{u}^2}{2\theta} \right] \\
&= w_\alpha \sum_{n=0}^N \frac{H_n(\xi_\alpha)}{n!} \left(\frac{\mathbf{u}}{\sqrt{2\theta}} \right)^n \quad (28)
\end{aligned}$$

where $\xi_\alpha \equiv \mathbf{c}_\alpha \cdot \hat{\mathbf{u}}/\sqrt{2\theta}$. Hence the task to prove Theorem 2 is to prove $\tilde{\mathbf{M}}^{(n)}$ ($\forall n \leq N$) generated by $f_\alpha^{eq, (N)}$ is equal to $\mathbf{M}^{(n)}$ from the full Maxwell-Boltzmann distribution f^{eq} or its truncation $f^{eq, (N)}$. According to definition (1), we have

$$\begin{aligned}
\mathbf{M}^{(n)} &\equiv \int d^D \mathbf{c} \underbrace{\mathbf{c} \cdots \mathbf{c}}_n f^{eq}(\mathbf{x}, \mathbf{c}, t) \\
&= \frac{1}{(2\pi\theta)^{D/2}} \sum_{n=0}^N \frac{1}{n!} \left(\frac{\mathbf{u}}{\sqrt{2\theta}} \right)^n \\
&\quad \times \int d^D \mathbf{c} \underbrace{\mathbf{c} \cdots \mathbf{c}}_n \exp \left[-\frac{\mathbf{c}^2}{2\theta} \right] H_n(\xi) \quad (29)
\end{aligned}$$

On the other hand, according to (5), we have

$$\begin{aligned}\tilde{\mathbf{M}}^{(n)} &\equiv \sum_{i=0}^b \underbrace{\mathbf{c}_\alpha \cdots \mathbf{c}_\alpha}_n f_\alpha^{eq, (N)} \\ &= \sum_{n=0}^N \frac{1}{n!} \left(\frac{\mathbf{u}}{\sqrt{2\theta}} \right)^n \sum_{\alpha=0}^b \underbrace{\mathbf{c}_\alpha \cdots \mathbf{c}_\alpha}_n w_\alpha H_n(\xi_\alpha) \quad (30)\end{aligned}$$

From (29) and (30), we see that both of these involve Hermite polynomials of orders no greater than N . Furthermore, a given Hermite function $H_n(x)$ is a polynomial of x^m ($m = 0, \dots, \leq n$). Therefore, both $\mathbf{M}^{(n)}$ and $\tilde{\mathbf{M}}^{(n)}$ involve powers of \mathbf{c} (or \mathbf{c}_α) from 0 up to $n + N$. Based this observation, we see that it is sufficient to prove $\tilde{\mathbf{M}}^{(n)} = \mathbf{M}^{(n)}$ ($\forall n \leq N$), if for all integer $m \leq 2N$ the following property is satisfied,

$$\int d^D \mathbf{c} \frac{\exp[-\mathbf{c}^2/2\theta]}{(2\pi\theta)^{D/2}} \underbrace{\mathbf{c} \cdots \mathbf{c}}_m = \sum_{\alpha=0}^b w_\alpha \underbrace{\mathbf{c}_\alpha \cdots \mathbf{c}_\alpha}_m \quad (31)$$

$$\forall m = 0, \dots, 2N$$

The result for the discrete summation is already given in the definition of (11) and (24). Hence it is suffice to just show that this is also true for the continuum integration. In fact, according to the basic Gaussian integral property, we know that

$$\begin{aligned}&\frac{1}{(2\pi\theta)^{D/2}} \int d^D \mathbf{c} \exp \left[-\frac{\mathbf{c}^2}{2\theta} \right] c_{i_1} c_{i_2} \cdots c_{i_m} \\ &= \begin{cases} \theta^{m/2} \Delta_{i_1, i_2, \dots, i_m}^{(m)}, & m = 0, 2, 4, \dots, 2N \\ 0, & m = 1, 3, 5, \dots, 2N + 1 \end{cases} \quad (32)\end{aligned}$$

Consequently, we have proved $\tilde{\mathbf{M}}^{(n)} = \mathbf{M}^{(n)}$ ($\forall n \leq N$), and thus Theorem 2.

It is also worthwhile to note, without repeating the explicit steps of the above, that the same proof applies if the truncation of the exponential form f_α^{eq} is up to $N + 1$. Thus, we can retain an extra term in the expanded form.

4. Discussion

In this paper, we have presented and proved a set of fundamental conditions for formulating LBM models. Lattice velocity sets obeying these conditions automatically produce equilibrium moment accuracy to any given N -th order. As demonstrated in [5], non-equilibrium moments are theoretically expressible as spatial and temporal derivatives of equilibrium moments. Therefore, achieving higher

order moment accuracy enables accurate description of fluid properties into deeper non-equilibrium regimes [21,22]. This is essential for physical properties at finite Knudsen or Mach numbers that are beyond the Navier-Stokes representation.

To make a more direct comparison with conventional LBM models, we rewrite (28) in a more explicit form (up to $O(u^5)$) below,

$$\begin{aligned}f_\alpha^{eq} &= w_\alpha \rho \left[1 + \frac{\mathbf{c}_\alpha \cdot \mathbf{u}}{\theta} + \frac{(\mathbf{c}_\alpha \cdot \mathbf{u})^2}{2\theta^2} - \frac{\mathbf{u}^2}{2\theta} \right. \\ &\quad + \frac{(\mathbf{c}_\alpha \cdot \mathbf{u})^3}{6\theta^3} - \frac{(\mathbf{c}_\alpha \cdot \mathbf{u})\mathbf{u}^2}{2\theta^2} \\ &\quad + \frac{(\mathbf{c}_\alpha \cdot \mathbf{u})^4}{24\theta^4} - \frac{(\mathbf{c}_\alpha \cdot \mathbf{u})^2\mathbf{u}^2}{4\theta^3} + \frac{\mathbf{u}^4}{8\theta^2} \\ &\quad \left. + \frac{(\mathbf{c}_\alpha \cdot \mathbf{u})^5}{120\theta^5} - \frac{(\mathbf{c}_\alpha \cdot \mathbf{u})^3\mathbf{u}^2}{12\theta^4} + \frac{(\mathbf{c}_\alpha \cdot \mathbf{u})\mathbf{u}^4}{8\theta^3} \right] \quad (33)\end{aligned}$$

It is immediately recognized that the series for most of the conventional LBM models terminate at $O(u^2)$ or $O(u^3)$. For example, the so called D3Q15 and D3Q19 correspond to the expansion up to $O(u^2)$ [14]. It can be directly verified that their underlying lattice velocity sets only satisfy the fundamental conditions (24) up to $N = 2$, so that the higher order moment terms beyond $O(u^3)$ can not be accurately supported. Furthermore, in these models, the temperature is fixed at $\theta = 1/3$. An extended 34-velocity model exists [17,23], and its temperature has a range of variation between $1/3$ to $2/3$, and D3Q19 is its reduced limit as $\theta = 1/3$. But the moment accuracy is still $N = 2$.

There are typically two approaches to construct lattice velocity sets obeying higher order of accuracies ($N > 2$) according to (24). One approach is to rely on relations between discrete rotational symmetry and tensor isotropy [11,24]. For instance, we can start with a lattice velocity set consisting of multiple lattice speeds, namely

$$\mathcal{L} = \mathcal{L}_1 \cup \mathcal{L}_2 \cdots \cup \mathcal{L}_M \quad (34)$$

where each of the subset is defined as

$$\mathcal{L}_\beta = \{\mathbf{c}_{\alpha,\beta}; i = 0, \dots, b_\beta\}$$

$$\beta = 1, \dots, M$$

All lattice velocities in each subset \mathcal{L}_β has the same magnitude, $|\mathbf{c}_{\alpha,\beta}| = c_\beta$. This way, the required isotropy can be imposed at each speed level. It has been shown that if such a velocity subset is parity invariant and obeys an n -th order isotropy

($n = \text{even integer}$), then its basic moment tensor has the following form [24]

$$\mathbf{E}_{i_1, i_2, \dots, i_n}^{(n), \beta} = b_\beta c_\beta^n \frac{(D-2)!!}{(D+n-2)!!} \Delta_{i_1, i_2, \dots, i_n}^{(n)} \quad (35)$$

and it vanishes for all the odd integer moments. Subsequently, we can assign a weighting factor $w_\beta(\theta)$ for each subset \mathcal{L}_β , so that the overall condition (24) is achieved by satisfying the following constraint on the weighting factors,

$$\sum_{\beta=1}^M b_\beta c_\beta^n \frac{(D-2)!!}{(D+n-2)!!} w_\beta(\theta) = \theta^{n/2} \quad (36)$$

for $n = 0, 2, \dots, 2N$. There are $2N + 1$ such constraints. Hence, it is necessary to include enough number of subsets and $w_\beta(\theta)$ ($\beta = 1, \dots, M \geq N + 1$) in order to have a solution. Using such a procedure, a 59-velocity model in 3-dimension is formulated that satisfies (24) up to $N = 3$ with 6-th order tensor isotropy, so that the expansion in (33) can be carried to $O(u^4)$. Based on the analysis above and else where [5], such an order of moment accuracy is necessary for getting the correct energy flux in thermal hydrodynamics [25,26,27]. Another approach is to form the discrete velocity sets via Gaussian quadrature for higher order models [5]. Indeed, (32) defines the precise requirement. The only difference here is that the quadratures need to allow a variable temperature θ . This approach is relatively more straightforward, so that it enables a systematic formulation of higher accurate LBM models to 6-th, 8-th orders and beyond. There is also a similar work recently by Sbragaglia et al on how to construct higher order isotropic moments [28].

The formulation described in this paper offers a rigorous measure for evaluating the order of accuracy of a given LBM model. For future convenience, we may simply refer an LBM model that satisfies condition (24) to N -th order as “E(N)-accurate.”

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